Succinic acid, hex-4-yn-3-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C19H24O5/c1-5-9-15(6-2)23-18(20)12-13-19(21)24-17-11-8-7-10-16(17)22-14

InchiKey: MPKMSXPTBGPUBR-UHFFFAOYSA-N

Formula: C19H24O5

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 332.39

Physical Properties

Property code	Value	Unit	Source
gf	-163.04	kJ/mol	Joback Method
hf	-570.51	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.505		Crippen Method
mcvol	266.960	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2285.00		NIST Webbook
tb	848.90	K	Joback Method
tc	1066.67	K	Joback Method
tf	585.48	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.43	J/mol×K	848.90	Joback Method
cpg	812.44	J/mol×K	885.20	Joback Method
cpg	826.17	J/mol×K	921.49	Joback Method
cpg	838.62	J/mol×K	957.79	Joback Method
cpg	849.78	J/mol×K	994.08	Joback Method
cpg	859.67	J/mol×K	1030.38	Joback Method
cpg	868.28	J/mol×K	1066.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389791&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume